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The maximum Wiener polarity index of trees with k pendants☆

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ABSTRACT

The Wiener polarity index $W_p(G)$ of a graph $G = (V, E)$ is the number of unordered pairs of vertices $\{u, v\}$ of G such that the distance $d_G(u, v)$ between u and v is 3. In this work, we give the maximum Wiener polarity index of trees with n vertices and k pendants and find that the maximum value is independent of k when $k + 2 \leq n \leq 2k$. The corresponding extremal trees are characterized.

1. Introduction

The Wiener polarity index of an organic molecule whose molecular graph is $G = (V, E)$ is defined (see [1,2]) as

$$W_P(G) = |\{\{u, v\}|d_G(u, v) = 3, u, v \in V\}|$$

which is the number of unordered pairs of vertices $\{u, v\}$ of G such that $d_G(u, v) = 3$, where $d_G(u, v)$ is the distance between two vertices u and v in G.

Using the Wiener polarity index, Lukovits and Linert [3] demonstrated quantitative structure–property relationships in a series of acyclic and cycle-containing hydrocarbons. Hosoya [4] found a physico-chemical interpretation of $W_P(G)$. Very recently, Du, Li and Shi [1] described a linear time algorithm APT for computing the index of trees, and characterized the trees maximizing the index among all trees of given order. Deng, Xiao and Tang [2] characterized the extremal trees with respect to this index among all trees of order n and diameter d. Deng [5] gave the extremal Wiener polarity indices of all chemical trees with order n. Xiao and Deng [6] found the maximum Wiener polarity index of chemical trees with n vertices and k pendants. Tong and Deng [7] characterized the trees with the first three smallest Wiener polarity indices among all trees of order n and diameter d. Mathematical properties of the Wiener polarity index and its applications in chemistry can be found in [1–5] and the references cited therein.

In this work, we further consider the Wiener polarity indices of trees. The maximum Wiener polarity index of trees with n vertices and k pendants is obtained and the corresponding extremal trees are characterized.

2. Some properties of the Wiener polarity index

Let T be a tree with its vertex set $V(T)$ and edge set $E(T)$. We denote by $N_T(v)$ the set of neighbors of v, and by $d_T(v) = |N_T(v)|$ the degree of a vertex $v \in V(T)$. A path P in T is called an i-degree pendant chain (or simply, a pendant chain) if all

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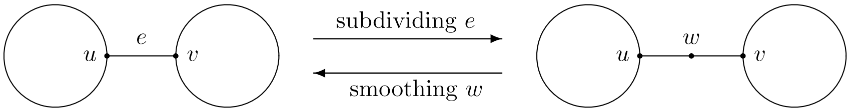

Fig. 1. The operations of subdividing and smoothing.

of its internal vertices are of degree 2 and its ends of degree 1 and i respectively, where $i \geq 3$. In particular, P is called an i-degree pendant edge if P is an edge. A tree T is called a star-like tree if all of its vertices except one are of degree 1 or 2. For convenience, let $\mathcal{T}_n$ be the set of trees of order n and $\mathcal{T}_{n,k}$ the set of trees of order n with k pendants.

We first give a formula for computing the Wiener polarity index of trees.

Lemma 1 ([1,2]). *Let $T = (V, E)$ be a tree. Then*

$$W_p(T) = \sum_{uv \in E} (d_T(u) - 1)(d_T(v) - 1). \quad \square$$

Let m_{ij} be the number of edges in T between vertices of degrees i and j. By Lemma 1, we have

$$W_p(T) = \sum_{uv \in E(T)} (d_T(u) - 1)(d_T(v) - 1) = \sum_{1 \leq i \leq j \leq n-1} (i-1)(j-1)m_{ij}.$$

Now, we introduce two graph transformations which will be used in the next section.

An edge $e = uv$ is said to be subdivided when it is deleted and replaced by a path of length 2 connecting u and v, the internal vertex w of this path being a new vertex. The converse of subdividing is called smoothing the vertex w of degree 2. This is illustrated in Fig. 1.

The following two lemmas can be proved by direct computation from Lemma 1.

Lemma 2. *Let us have $T \in \mathcal{T}_n$. $e = uv$ is an edge of T with $d_T(u) \leq d_T(v)$. T' is the tree obtained by subdividing e. Then*

$$W_p(T') - W_p(T) \begin{cases} = d_T(v) - 1, & d_T(u) = 1; \\ = 1, & d_T(u) = 2; \\ = 3 - d_T(v), & d_T(u) = 3; \\ < 0, & d_T(u) \geq 4. \end{cases}$$

Proof. By Lemma 1, we have

$$W_p(T') - W_p(T) = d_T(u) - 1 + d_T(v) - 1 - (d_T(u) - 1)(d_T(v) - 1).$$

Since $d_T(v) \geq d_T(u)$, Lemma 2 is an immediate result from the formula above. $\square$

Similarly, we have:

Lemma 3. *Let us have $T \in \mathcal{T}_n$. w is a vertex of degree 2 of T whose neighbors are u and v, $d_T(u) \leq d_T(v)$. T' is the tree obtained by smoothing w. Then*

$$W_p(T') - W_p(T) \begin{cases} = 1 - d_T(v), & d_T(u) = 1; \\ = -1, & d_T(u) = 2; \\ = d_T(v) - 3, & d_T(u) = 3; \\ > 0, & d_T(u) \geq 4. \end{cases} \quad \square$$

Lemma 4. *Let us have $T \in \mathcal{T}_{n,k}$, $e = uv$ an edge of T with $d_T(u) = p + 1 \geq 3$ and $d_T(v) = q + 1 \geq 3$, and $T' = T/e$ the tree obtained by contracting e (see Fig. 2). If the degrees of all the neighbors of u and v are at least 2, then $W_p(T) \leq W_p(T')$.*

Proof. Let $X = N_T(u) - \{v\}$ and $Y = N_T(v) - \{u\}$. By Lemma 1,

$$\begin{aligned} W_p(T') - W_p(T) &= \sum_{x \in X} (d_T(x) - 1)(p + q - 1) + \sum_{y \in Y} (d_T(y) - 1)(p + q - 1) \\ &\quad - \sum_{x \in X} (d_T(x) - 1)p - \sum_{y \in Y} (d_T(y) - 1)q - pq \\ &= \sum_{x \in X} (d_T(x) - 1)(q - 1) + \sum_{y \in Y} (d_T(y) - 1)(p - 1) - pq \\ &\geq (q - 1)p + (p - 1)q - pq \\ &= pq - p - q \geq 0. \quad \square \end{aligned}$$

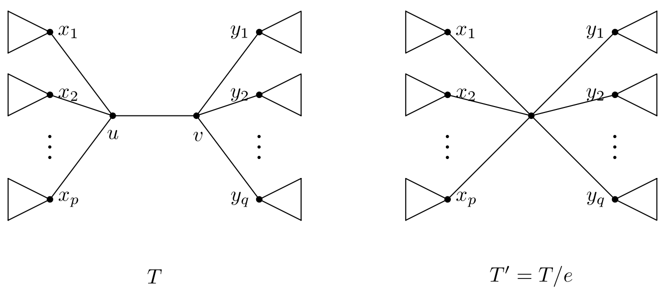

Fig. 2. The graphs in Lemma 4.

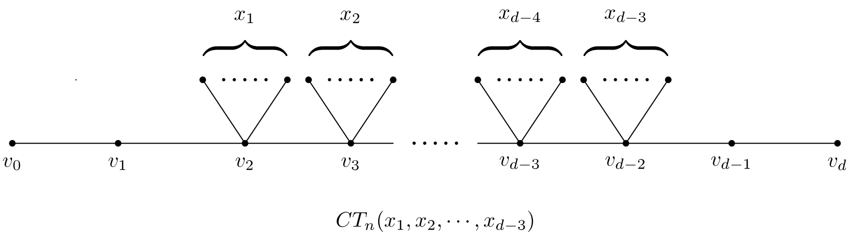

Fig. 3. The caterpillar tree $CT_n(x_1, x_2, \ldots, x_{d-3})$.

Let $CT_n(x_1, x_2, \ldots, x_{d-3})$ be a caterpillar tree with diameter d depicted in Fig. 3, where $x_1 + x_2 + \cdots + x_{d-3} = n - d - 1$. The following result is Theorem 7 in [2].

Lemma 5 *([2]). If $T \in \mathcal{T}_n$ with diameter $d \geq 5$, then*

$$W_p(T) \leq \left\lfloor \frac{n-d-1}{2} \right\rfloor \left\lceil \frac{n-d-1}{2} \right\rceil + (2n - d - 4)$$

with equality if and only if T is a caterpillar tree $CT_n(0, \ldots, 0, x_i, x_{i+1}, x_{i+2}, 0, \ldots, 0)$ such that where $1 \leq i \leq d-5$, $x_i + x_{i+1} + x_{i+2} = n - d - 1$, $x_i \geq 0$, $x_{i+2} \geq 0$ and $x_{i+1} = \left\lfloor \frac{n-d-1}{2} \right\rfloor$ or $\left\lceil \frac{n-d-1}{2} \right\rceil$. $\square$

3. The maximum Wiener polarity index of trees with *n* vertices and *k* pendants

In this section, we will discuss the maximum Wiener polarity index of trees with n vertices and k pendants.

We first consider some special cases. Let us have $T \in \mathcal{T}_n$ with diameter d.

If $k = 2$, then T is the path P_n with order n, and $W_p(P_n) = n - 3$ for $n \geq 4$ and $W_p(P_n) = 0$ for $n = 2, 3$.

If $k = n - 1$ or $d = 2$, then T is the star S_n with order n, and $W_p(S_n) = 0$.

If $k = n - 2$ or $d = 3$, then T is a double star. And $W_p(T) \leq \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil$ with equality if and only if T is the double star obtained by connecting the centers of stars $S_{\lfloor \frac{n}{2} \rfloor}$ and $S_{\lceil \frac{n}{2} \rceil}$.

In the following, we assume that $3 \leq k \leq n - 3$ and $d \geq 4$, and distinguish the following two cases.

Case I. $k + 3 \leq n \leq 2k$.

Let us have $T \in \mathcal{T}_{n,k}$ with diameter 4. It is not difficult to see [1] that $T = T(k_1, k_2, k_3, l_1, l_2, \ldots, l_m)$ can be represented by $m + 3$ integers $k_1, k_2, k_3, l_1, l_2, \ldots, l_m$ (see Fig. 4), where $k_i \geq 0$ $(i = 1, 2, 3)$, $m \geq 0$, $l_j \geq 1$ $(1 \leq j \leq m)$ when $m \geq 1$, and

$$k_1 + k_2 + k_3 + l_1 + l_2 + \cdots + l_m = n - m - 5.$$

The following Lemma 6 can be easily obtained from [1]; its proof is omitted here.

Lemma 6. *Let us have $T \in \mathcal{T}_{n,k}$ $(k + 3 \leq n \leq 2k)$ with diameter 4. Then*

$$W_p(T) \leq \begin{cases} \dfrac{n^2}{4} - n + \dfrac{3}{4}, & n \text{ is odd;} \\ \dfrac{n^2}{4} - n + 1, & n \text{ is even} \end{cases}$$

with equality if and only if $k_2 = k + 1 - \left\lfloor \frac{n}{2} \right\rfloor$ or $k_2 = k + 1 - \left\lceil \frac{n}{2} \right\rceil$. $\square$

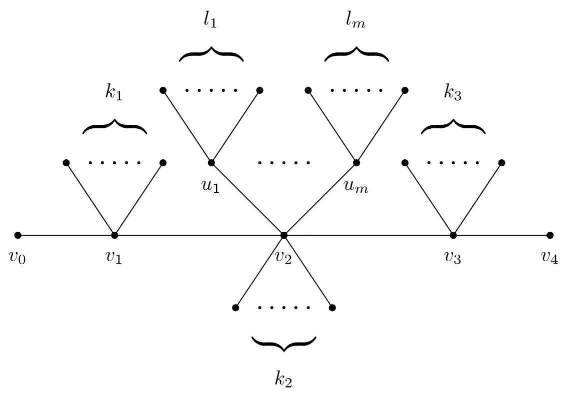

Fig. 4.

Lemma 7. *Let us have $T \in \mathcal{T}_{n,k}$ $(k+3 \le n \le 2k)$ with diameter $d \ge 5$. Then $W_p(T) < \frac{n^2}{4} - n + \frac{3}{4}$.*

Proof. By Lemma 5, we have

$$W_p(T) \le \left\lfloor \frac{n-d-1}{2} \right\rfloor \left\lceil \frac{n-d-1}{2} \right\rceil + (2n-d-4) = f(d)$$

$$f(d) = \begin{cases} \left(\frac{n-d-2}{2}\right)\left(\frac{n-d}{2}\right) + (2n-d-4), & n-d-1 \text{ is odd;} \\ \left(\frac{n-d-1}{2}\right)^2 + (2n-d-4), & n-d-1 \text{ is even} \end{cases}$$

and $f(5) = \frac{n^2}{4} - n - \frac{1}{4}$ or $\frac{n^2}{4} - n$. Since f is decreasing, $f(d) \le f(5) < \frac{n^2}{4} - n + \frac{3}{4}$. So, $W_p(T) < \frac{n^2}{4} - n + \frac{3}{4}$. $\square$

From Fig. 4, we know that $k_1 + k_2 + k_3 + l_1 + l_2 + \cdots + l_m = k-2$ and $k_1 + k_2 + k_3 + l_1 + l_2 + \cdots + l_m = n-m-5$. Since $0 \le m \le k-2$, $n-k-3 \le k-2 \le n-5$, i.e., $k+3 \le n \le 2k+1$. Conversely, for $k+3 \le n \le 2k+1$, i.e., $n-k-3 \le k-2 \le n-5$, there is $0 \le m \le k-2$ such that $k-2 = n-m-5$ and $T = T(k_1, k_2, k_3, l_1, l_2, \ldots, l_m)$ is a tree of diameter 4 with n vertices and k pendants, where $k_1 = k-2-m$, $k_2 = k_3 = 0$, $l_1 = \cdots = l_m = 1$. So, there is a tree of diameter 4 with n vertices and k pendants for $k+3 \le n \le 2k+1$. Among all trees of n vertices and k pendants with $k+3 \le n \le 2k$, we only need to consider the maximum Wiener polarity index of trees with diameter 3 or 4.

Summarizing Lemmas 6 and 7 and the case $k = n-2$ above, we have:

Theorem 1. *Let us have $T \in \mathcal{T}_{n,k}$ $(k+2 \le n \le 2k)$ with $n \ge 4$. Then*

$$W_p(T) \le \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil = \begin{cases} \frac{n^2}{4} - n + \frac{3}{4}, & n \text{ is odd;} \\ \frac{n^2}{4} - n + 1, & n \text{ is even} \end{cases}$$

with equality if and only if (i) *$T = T(k_1, k_2, k_3, l_1, \ldots, l_m)$ with $k_2 = k+1-\lfloor \frac{n}{2} \rfloor$ or $k_2 = k+1-\lceil \frac{n}{2} \rceil$, or* (ii) *$T$ is the double star obtained by connecting the centers of stars $S_{\lfloor \frac{n}{2} \rfloor}$ and $S_{\lceil \frac{n}{2} \rceil}$.* $\square$

This result shows that the maximum Wiener polarity index is independent of k when $k+2 \le n \le 2k$.

Case II. $n \ge 2k+1$.

Theorem 2. *Let us have $T \in \mathcal{T}_{n,k}$ $(n \ge 2k+1)$. Then*

$$W_p(T) \le k^2 - 3k + n - 1$$

with equality if and only if T is a star-like tree of order n in which the lengths of all pendant chains are at least 2.

Proof. By Lemma 1, we have $W_p(T) = k^2 - 3k + n - 1$ for any star-like tree T with n vertices and k pendants in which the lengths of all pendant chains are at least 2.

Suppose T is a tree with the maximum Wiener polarity index among all trees of n vertices and k pendants ($n \geq 2k+1$).

(i) First, all vertices of degree 2 in T are on the pendant chains of T.

Otherwise, there is a path $xv_1 \cdots v_t y$ in T such that $d_T(x) \geq 3$, $d_T(y) \geq 3$, $d_T(v_1) = \cdots = d_T(v_t) = 2$ and $t \geq 1$. Let T_1 be the tree obtained by smoothing the vertices $v_1, \ldots, v_t$; then

$$W_p(T_1) = W_p(T) + (d_T(x)-1)(d_T(y)-1) - ((d_T(x)-1) + (t-1) + (d_T(y)-1)).$$

Let T_2 be obtained from T_1 by subdividing a pendant edge $e = uv$ (where v is a pendant vertex and $d_T(u) \geq 2$) t times, i.e., inserting n vertices $v_1, \ldots, v_t$ into the edge e. Then $T_2 \in \mathcal{T}_{n,k}$ and

$$W_p(T_2) = W_p(T_1) + (d_T(u)-1) + (t-1).$$

So,

$$\begin{aligned} W_p(T_2) &= W_p(T) + (d_T(x)-1)(d_T(y)-1) - ((d_T(x)-1) + (d_T(y)-1)) + d_T(u) - 1 \\ &= W_p(T) + \left(\frac{1}{2}(d_T(x)-1) - 1\right)(d_T(y)-1) + \left(\frac{1}{2}(d_T(y)-1) - 1\right)(d_T(x)-1) + d_T(u) - 1 \\ &\geq W_p(T) + d_T(u) - 1 \\ &\geq W_p(T) + 1, \end{aligned}$$

a contradiction.

(ii) Secondly, if T has a i-degree pendant edge with $i \geq 3$, then the length of each pendant chain in T is at most 2.

Otherwise, there is a pendant chain Q_1 of length $l \geq 3$ and a i-degree pendant edge Q_2, $i \geq 3$. Smoothing one of vertices with degree 2 on Q_1 and subdividing the pendant edge on Q_2, we obtain a tree $T_3 \in \mathcal{T}_{n,k}$. By Lemmas 2 and 3, $W_p(T_3) = W_p(T) - 1 + (i-1) > W_p(T)$, a contradiction.

(iii) Finally, we prove that T is a star-like tree of order n in which the lengths of all pendant chains are at least 2.

We denote by $n_2 = n_2(T)$ the number of vertices with degree 2 in T.

If $n_2 < k$, then there are exactly $k - n_2$ i-degree pendant edges such that $i \geq 3$ in T from (ii). Let T_4 be the tree obtained by subdividing these i-degree pendant edges. We have $T_4 \in \mathcal{T}_{n+k-n_2,k}$ and $W_p(T_4) > W_p(T)$. Now, there are $(n+k-n_2-1) - 2k = n-k-n_2-1$ edges whose ends have degrees greater than two in T_4 since there are exactly $2k$ edges on the pendant chains. If T_5 is obtained by contracting these edges from T_4, then $T_5 \in \mathcal{T}_{2k+1,k}$ is a star-like tree of order $2k+1$ and $W_p(T_5) \geq W_p(T_4)$ by Lemma 4. Let T_6 be the tree obtained by inserting $n-(2k+1)$ vertices into an edge of T_5. Then $T_6 \in \mathcal{T}_{n,k}$ is a star-like tree of order n and $W_p(T_6) > W_p(T_5)$ by Lemma 2. And $W_p(T_6) > W_p(T)$, a contradiction.

So, $n_2 \geq k$, and the lengths of all pendant chains in T are at least 2 from (i) and (ii). If T is not a star-like tree, let r be the number of edges whose ends have degrees greater than 2, so we have $r \geq 1$.

If T_7 is obtained by contracting the r edges from T, then $T_7 \in \mathcal{T}_{n-r,k}$ is a star-like tree of order $n-r$ and $W_p(T_7) \geq W_p(T)$ by Lemma 4. Let T_8 be the tree obtained by inserting r vertices into an edge of T_7; then $T_8 \in \mathcal{T}_{n,k}$ is a star-like tree of order n and $W_p(T_8) > W_p(T_7)$ by Lemma 2. Therefore $W_p(T_8) > W_p(T)$, a contradiction again. $\square$

From Theorems 1 and 2, we have:

Corollary 1. *Among all trees with n vertices and k pendants, the maximum Wiener polarity index is*

$$W_p(T)_{\max} = \begin{cases} 0, & n = k+1; \\ \left\lfloor \dfrac{n-2}{2} \right\rfloor \left\lceil \dfrac{n-2}{2} \right\rceil, & k+2 \leq n \leq 2k; \\ k^2 - 3k + n - 1, & n \geq 2k+1. \end{cases} \quad \square$$

Since $k^2 - 3k + n - 1 \leq \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil$ when $n \geq 2k+1$, we obtain the following result:

Corollary 2 ([1]). *Among all trees of order $n \geq 4$, a tree T has the maximal Wiener polarity index if and only if $W_p(T) = \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil$, and* (i) *$T = T(k_1, k_2, k_3, l_1, \ldots, l_m)$ with $k_2 = k + 1 - \left\lfloor \frac{n}{2} \right\rfloor$ or $k_2 = k + 1 - \left\lceil \frac{n}{2} \right\rceil$, or* (ii) *$T$ is the double star obtained by connecting the centers of stars $S_{\lfloor \frac{n}{2} \rfloor}$ and $S_{\lceil \frac{n}{2} \rceil}$.* $\square$

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